

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.58

Global applicability domain: Inside

Local applicability domain index: 5.78e-01

Confidence level: 6.33e-01

Nearest Neighbors from the Training Set

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tert-Butyl alcohol

Measured: 5.01

Predicted: 4.48

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Diethyl ether

Measured: 5.37

Predicted: 4.72

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Methyl tert-butyl ether

Measured: 1.51

Predicted: 3.67

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4-Methylimidazolidine-2-thione

Measured: 10.0

Predicted: 4.59

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Triethylamine

Measured: 4.90

Predicted: 5.95